Italicen-12-yl isobutyrate

Inchi: InChI=1S/C19H30O2/c1-12(2)17(20)21-11-18(5)15-7-6-14(4)19(15)9-8-13(3)10-16(18)19
InchiKey: QSRNPZUAEPFPOS-DZBHQSCQSA-N
Formula: C19H30O2
SMILES: CC1=CC2C(C)(COC(=O)C(C)C)C3CCC(C)C23CC1
Mol. weight [g/mol]: 290.44

Physical Properties

Property code	Value	Unit	Source
gf	24.72	kJ/mol	Joback Method
hf	-443.38	kJ/mol	Joback Method
hfus	24.81	kJ/mol	Joback Method
hvap	64.77	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.594		Crippen Method
mcvol	249.130	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	1910.00		NIST Webbook
tb	734.01	K	Joback Method
tc	952.22	K	Joback Method
tf	460.43	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.83	J/mol×K	734.01	Joback Method
cpg	806.18	J/mol×K	770.38	Joback Method
cpg	827.92	J/mol×K	806.75	Joback Method
cpg	849.32	J/mol×K	843.12	Joback Method
cpg	870.63	J/mol×K	879.48	Joback Method
cpg	892.13	J/mol×K	915.85	Joback Method
cpg	914.08	J/mol×K	952.22	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R233177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume